

Adiabatic theorems for linear and nonlinear Hamiltonians

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Abstract

Conditions for the validity of the quantum adiabatic approximation are analyzed. For the case of linear Hamiltonians, a simple and general sufficient condition is derived, which is valid for arbitrary spectra and any kind of time variation. It is shown that in some cases the found condition is necessary and sufficient. The adiabatic theorem is generalized for the case of nonlinear Hamiltonians.

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1 Introduction

The quantum adiabatic theorem is one of the principal results in quantum mechanics [1]. The standard consideration assumes a quantum system, whose Hamiltonian $H(t)$ varies slowly in time [1,2]. The wave function satisfies the Schrödinger equation

$$i\dot{\psi}(t) = H(t) \psi(t) , \quad (1)$$

where the overdot, as usual, implies time differentiation. Here and in what follows, the system of units is employed, where $\hbar = 1$. For the sake of compactness, the matrix notation is employed, when the wave function is treated as a vector-column with respect to its spatial, spin, and other variables, except time t ; and the Hamiltonian is a matrix in these variables. The wave function is normalized to one, $||\psi(t)|| = 1$, with the Euclidean vector norm assumed. The system Hamiltonian contains an explicit dependence on time.

Keeping time as a parameter, one considers the eigenproblem

$$H(t) \psi_n(t) = E_n(t) \psi_n(t) . \quad (2)$$

The eigenfunctions are normalized to one, $||\psi_n(t)|| = 1$. The multi-index n , in general, can pertain to a discrete or continuous set.

If at the initial time $t = 0$ the system starts from a state

$$\psi(0) = \psi_j(t) , \quad (3)$$

with a fixed j , and the Hamiltonian variation is sufficiently slow, then at the moment t it is in a state that is close to $\psi_j(t)$. This, roughly speaking, is the meaning of the adiabatic theorem (see details in Refs. [1,2]). The criterion on the slowness, required by the theorem, is often formulated [3,4] as the inequality

$$\left| \frac{\langle \psi_n(t) | \dot{\psi}_j(t) \rangle}{E_{nj}(t)} \right| \ll 1 \quad (n \neq j) \quad (4)$$

that is to be valid for all $n \neq j$, in the time interval $[0, \tau]$. Here

$$E_{mn}(t) \equiv E_m(t) - E_n(t) .$$

By differentiating Eq. (2), one gets

$$\dot{E}_n(t) = \langle \psi_n(t) | \dot{H}(t) | \psi_n(t) \rangle ,$$

$$E_{mn}(t) \langle \psi_m(t) | \dot{\psi}_n(t) \rangle = - \langle \psi_m(t) | \dot{H}(t) | \psi_n(t) \rangle ,$$

which allows to rewrite condition (4) in another form

$$\left| \frac{\langle \psi_n(t) | \dot{H}(t) | \psi_j(t) \rangle}{E_{nj}^2(t)} \right| \ll 1 \quad (n \neq j) . \quad (5)$$

As is evident, conditions (4) or (5) have sense only when the denominator $E_{nj} \neq 0$. This imposes the restrictions on the spectrum of the considered system: The spectrum has to be nondegenerate; there should be no level crossings; and the fixed level j has to be separated

by a gap from other levels. Also, the requirement of the slow temporal variation of the Hamiltonian presupposes that the resonance case has to be excluded. This means that, if the effective frequency of the Hamiltonian variation is ω , than it has to be smaller than any of the transition frequencies $E_{mn}(t)$ (see discussion in Ref. [6]).

Moreover, conditions (4) or (5) are neither necessary nor sufficient. Thus, Messiah [4] mentions that such conditions are probably valid "in most cases". Since these conditions are not sufficient, their validity does not guarantee the applicability of the adiabatic approximation. Therefore, when such a condition holds but the adiabatic approximation fails, there is no any inconsistency in the adiabatic theorem. This trivial fact can be illustrated by a number of examples [5-10] and checked experimentally [11].

There exist mathematically correct formulations of the adiabatic theorem, relaxing some of the requirements on the spectrum. Thus, Born and Fock [1] considered the case with level crossings. Avron and Elgart [12] proved the theorem without a gap condition. There have been considered the variants of the adiabatic theorem for open systems [13], in the presence of noise [14], as well as corrections to the adiabatic approximation [15]. This interest to formulating convenient conditions for the validity of the adiabatic approximation is supported by the recent discussions on the feasibility of adiabatic quantum computation [16,17].

In the present paper, a novel simple and, at the same time, very general sufficient condition for the validity of the adiabatic approximation is derived. This condition is valid for arbitrary spectra and for any time variation of the system Hamiltonian, which is not required to be slow. If the latter is fast, the adiabatic approximation is respectively limited in time. By an explicit illustration, it is shown that, in some cases, the suggested condition is both necessary and sufficient. The second aim of the present paper is to generalize the adiabatic theorem to the case of nonlinear Hamiltonians. Such Hamiltonians are met, e.g., in nonlinear optics and in the physics of cold atoms (see review articles [18-26]).

2 Linear Hamiltonians

This is the standard case of quantum mechanics. The linear Hamiltonian $H(t)$ is self-adjoint. The set $\{\psi_n(t)\}$ of the eigenfunctions of Eq. (2) forms a complete orthonormal basis, such that

$$\langle \psi_m(t) | \psi_n(t) \rangle = \delta_{mn} .$$

The solution to Eq. (1) can be expanded over this basis as

$$\psi(t) = \sum_n a_n(t) \exp\{i\chi_n(t)\} \psi_n(t) , \quad (6)$$

where the phase

$$\chi_n(t) = \delta_n(t) + \zeta_n(t) \quad (7)$$

is the sum of the dynamic and geometric phases, respectively:

$$\delta_n(t) \equiv - \int_0^t E_n(t') dt' , \quad \zeta_n(t) \equiv i \int_0^t \langle \psi_n(t') | \dot{\psi}_n(t') \rangle dt' . \quad (8)$$

We may note that

$$\langle \dot{\psi}_m(t) | \psi_n(t) \rangle = - \langle \psi_m(t) | \dot{\psi}_n(t) \rangle ,$$

which follows from differentiating the orthonormality condition. To be precise, let us give the definition of what will be called the adiabatic approximation.

Definition (*Adiabatic approximation*). The function

$$\tilde{\psi}_j(t) = a_j(t) \exp\{i\chi_j(t)\} \psi_j(t) \quad (9)$$

is the adiabatic approximation for the solution $\psi(t)$ of Eq. (1), with the initial condition (3), if and only if

$$\| \psi(t) - \tilde{\psi}_j(t) \| \ll 1, \quad (10)$$

where the Euclidean vector norm is assumed.

Inequality (10) tells us that the Euclidean distance between functions $\psi(t)$ and $\tilde{\psi}_j(t)$ is small. This inequality is the necessary and sufficient condition for function (9) to be called the adiabatic approximation.

Theorem 1. Let the Hamiltonian $H(t)$ be linear and self-adjoint, $\psi(t)$ be the solution to Eq. (1), with the initial condition (3), and let $\psi_n(t)$ be the solutions to eigenproblem (2), which are differentiable over time. Then function (9) is the adiabatic approximation, for the time interval $[0, \tau]$, in the sense of definition (10), if the condition

$$\sum_{n(\neq j)} \int_0^t | \langle \psi_j(t') | \dot{\psi}_n(t') \rangle | dt' \ll 1 \quad (11)$$

holds for all $t \in [0, \tau]$.

Proof. Substituting Eqs. (6) and (9) into the left-hand side of Eq. (10) gives

$$\| \psi(t) - \tilde{\psi}_j(t) \|^2 = 1 - |a_j(t)|^2. \quad (12)$$

Hence, the necessary and sufficient condition (10) takes the form

$$1 - |a_j(t)|^2 \ll 1. \quad (13)$$

Using expansion (6) in Eq. (1) yields the equation

$$\dot{a}_m(t) = - \sum_{n(\neq m)} a_n(t) \langle \psi_m(t) | \dot{\psi}_n(t) \rangle \exp\{-i\chi_{mn}(t)\}, \quad (14)$$

where

$$\chi_{mn}(t) \equiv \chi_m(t) - \chi_n(t). \quad (15)$$

From Eq. (14), it follows that

$$\frac{d}{dt} |a_m(t)|^2 = -2\text{Re} \sum_{n(\neq m)} a_m^*(t) a_n(t) \langle \psi_m(t) | \dot{\psi}_n(t) \rangle \exp\{-i\chi_{mn}(t)\}. \quad (16)$$

Integrating the latter equation results in

$$\begin{aligned} |a_m(t)|^2 &= |a_m(0)|^2 - \\ &- 2\text{Re} \sum_{n(\neq m)} \int_0^t a_m^*(t') a_n(t') \langle \psi_m(t') | \dot{\psi}_n(t') \rangle \exp\{-i\chi_{mn}(t')\} dt'. \end{aligned} \quad (17)$$

In view of the initial condition (3), one has

$$a_n(0) = \delta_{nj} . \quad (18)$$

Using this and setting $m = j$ in Eq. (17) gives

$$1 - |a_j(t)|^2 = 2\text{Re} \sum_{n(\neq j)} \int_0^t a_j^*(t') a_n(t') < \psi_j(t') | \dot{\psi}_n(t') > \exp\{-i\chi_{mj}(t')\} dt' . \quad (19)$$

The necessary and sufficient condition for the validity of the adiabatic approximation is that the right-hand side of Eq. (19) be small, in agreement with inequality (13). Majorizing this right-hand side, with taking into account that $|a_n(t)| \leq 1$, leads to

$$1 - |a_j(t)|^2 \leq 2 \sum_{n(\neq j)} \int_0^t | < \psi_j(t') | \dot{\psi}_n(t') > | dt' . \quad (20)$$

Therefore, for inequality (13) to hold, it is sufficient that condition (11) be valid. This concludes the proof.

Remark. The summation in above formulas is over the spectral multi-index n , whose nature can be arbitrary. If it pertains to a continuous set, then the summation should be understood as integration. That is, the theorem is valid for discrete as well as for continuous spectra. In proving the theorem, no restrictions have been imposed on the spectral properties. The spectrum can be arbitrary, whether discrete or continuous, nondegenerate or degenerate, gapful or gapless, without or with level crossings. The rate of the Hamiltonian temporal variation is also arbitrary, including the resonance case. So, the sufficient condition (11) seems to be more general than many other known sufficient conditions. The relation of this condition (11) to other conditions of close forms will be considered in detail in the concluding section Discussion.

3 Nonlinear Hamiltonians

Now, let us try to expand the adiabatic theorem to the case of nonlinear Hamiltonians, such as appear in the problem of cold atoms [18-26]. Let a nonlinear Hamiltonian

$$H(t) = H[\psi, t] = H[|\psi|, t] , \quad (21)$$

depending on $|\psi(t)|$, be gauge-invariant, such that it is invariant with respect to the gauge transformation

$$H[\psi e^{i\alpha}, t] = H[\psi, t] , \quad (22)$$

where α is real. This type of Hamiltonians is typical of coherent systems corresponding to Bose-Einstein condensate. The function $\psi(t)$ is normalized to one and satisfies the same equation (1). A particular case of the latter could be, e.g., the Gross-Pitaevskii equation that is a nonlinear Schrödinger equation. The same initial condition (3) is assumed.

In the place of the eigenvalue problem (2), we have

$$H[\psi_n, t] \psi_n(t) = E_n(t) \psi_n(t) . \quad (23)$$

The eigenfunctions can be chosen to be normalized to one. We look for the solution of Eq. (1) in the same form (6). Strictly speaking, a nonlinear equation can possess several types of solutions. But we can limit the consideration by the class of solutions representable in form (6), where

$$| a_n(t) | \leq 1 . \quad (24)$$

An important difference of the nonlinear case, as compared to the linear one, is that the Hamiltonian $H[\psi_n, t]$ is not Hermitian since

$$< \psi_m(t) | H[\psi_n, t] \psi_n(t) > \neq < H[\psi_n, t] \psi_m(t) | \psi_n(t) > ,$$

for $m \neq n$. As a consequence, the eigenfunctions $\psi_m(t)$ and $\psi_n(t)$ are not orthogonal for $m \neq n$. Also, the matrix elements of the quantity

$$\Delta_n(t) \equiv H(t) - E_n(t) \quad (25)$$

are not zero, that is,

$$< \psi_m(t) | \Delta_n(t) | \psi_n(t) > \neq 0 .$$

This essentially complicates the consideration and makes more cumbersome sufficient conditions for the validity of the adiabatic approximation.

Theorem 2. Let a nonlinear gauge-invariant Hamiltonian be defined by Eqs. (21) and (22) and let the eigenfunctions of the eigenproblem (23) be time-differentiable. Let function (6) be a solution to Eq. (1), under conditions (3) and (24). Then function (9) is the adiabatic approximation for the time interval $[0, \tau]$, in the sense of definition (10), provided that the following conditions hold:

$$\sum_{n(\neq j)} | < \psi_n(t) | \psi_j(t) > | \ll 1 , \quad (26)$$

$$\sum_{n(\neq j)} \int_0^t | < \psi_n(t') | \dot{\psi}_j(t') > | dt' \ll 1 , \quad (27)$$

$$\sum_n \int_0^t | < \psi_j(t') | \Delta_j(t') | \psi_n(t') > | dt' \ll 1 , \quad (28)$$

for all $t \in [0, \tau]$.

Proof. The left-hand side of inequality (10) now reads as

$$\begin{aligned} & \| \psi(t) - \tilde{\psi}_j(t) \| = 1 - | a_j(t) |^2 - \\ & - 2\text{Re} \sum_{n(\neq j)} a_j^*(t) a_n(t) < \psi_j(t) | \psi_n(t) > \exp\{i\chi_{nj}(t)\} . \end{aligned} \quad (29)$$

Majorizing the right-hand side of Eq. (29) gives

$$\| \psi(t) - \tilde{\psi}_j(t) \| \leq 1 - | a_j(t) |^2 + \sum_{n(\neq j)} | < \psi_j(t) | \psi_n(t) > | . \quad (30)$$

From here, it is seen that for inequality (10) to be true, it is sufficient that condition (13) be valid together with condition (26). One may notice that

$$1 - | a_j(t) |^2 = (1 - | a_j(t) |) (1 + | a_j(t) |) \leq 2(1 - | a_j(t) |) .$$

Therefore, instead of condition (13), it is sufficient to have the inequality

$$1 - |a_j(t)| \ll 1. \quad (31)$$

From Eq. (1), with function (6), we obtain

$$\begin{aligned} \dot{a}_m(t) = & - \sum_{n(\neq m)} \left[a_n(t) < \psi_m(t) \mid \dot{\psi}_n(t) > + \dot{a}_n(t) < \psi_m(t) \mid \psi_n(t) > \right] \exp\{-i\chi_{mn}(t)\} - \\ & - i \sum_n a_n(t) < \psi_m(t) \mid \Delta_n(t) \mid \psi_n(t) > \exp\{-i\chi_{mn}(t)\}. \end{aligned} \quad (32)$$

Due to the Hamiltonian gauge invariance (22), the eigenproblem (23) is invariant with respect to the gauge transformation

$$\psi_n(t) \rightarrow \psi_n(t) e^{i\alpha_n(t)},$$

where $\alpha_n(t)$ is real. This makes it possible to impose the Fock gauge calibration

$$< \psi_n(t) \mid \dot{\psi}_n(t) > = 0. \quad (33)$$

Then phase (7) becomes

$$\chi_n(t) = \delta_n(t) = - \int_0^t E_n(t') dt'. \quad (34)$$

Denoting the right-hand side of Eq. (32) by $R(t)$, we write

$$\dot{a}_m(t) \equiv R(t). \quad (35)$$

Integrating this equation, setting $m = j$, and using Eq. (18), we get

$$a_j(t) - 1 = \int_0^t R(t') dt'. \quad (36)$$

Rewriting the latter equation as

$$1 = a_j(t) - \int_0^t R(t') dt'$$

and majorizing here the right-hand side, we find

$$1 \leq |a_j(t)| + \int_0^t |R(t')| dt'. \quad (37)$$

This means that for the validity of Eq. (31), it is sufficient that the inequality

$$\int_0^t |R(t')| dt' \ll 1 \quad (38)$$

be valid. Integrating the right-hand side of Eq. (32), we invoke the integration by parts in the term

$$\begin{aligned} & \int_0^t \dot{a}_n(t') < \psi_m(t') \mid \psi_n(t') > \exp\{-i\chi_{mn}(t')\} dt' = \\ & = a_n(t) < \psi_m(t) \mid \psi_n(t) > \exp\{-i\chi_{mn}(t)\} - a_n(0) < \psi_m(0) \mid \psi_n(0) > \exp\{-i\chi_{mn}(0)\} - \end{aligned}$$

$$\begin{aligned}
& - \int_0^t a_n(t') \left[\langle \dot{\psi}_m(t') | \psi_n(t') \rangle + \langle \psi_m(t') | \dot{\psi}_n(t') \rangle + \right. \\
& \quad \left. + iE_{mn}(t') \langle \psi_m(t') | \psi_n(t') \rangle \right] \exp\{-i\chi_{mn}(t')\} dt' .
\end{aligned} \tag{39}$$

Then Eq. (37), with $R(t)$ given by the right-hand side of Eq. (32), yields

$$\begin{aligned}
1 - |a_j(t)| & \leq \sum_{n(\neq j)} [|\langle \psi_j(t) | \psi_n(t) \rangle| + |\langle \psi_j(0) | \psi_n(0) \rangle|] + \\
& + \sum_{n(\neq j)} \int_0^t |\langle \dot{\psi}_j(t') | \psi_n(t') \rangle| dt' + \sum_n \int_0^t |\langle \psi_j(t') | \Delta_j(t') | \psi_n(t') \rangle| dt' .
\end{aligned} \tag{40}$$

From here it becomes evident that inequality (31) holds, provided that conditions (26), (27), and (28) are satisfied. This concludes the proof.

4 Explicit illustration

To illustrate how the derived sufficient conditions work, it is reasonable to consider a simple case for which all calculations could be done explicitly and exactly. To this end, let us study the motion of a spin 1/2 in a rotating magnetic field [27]. The related magnetic moment is $\mathbf{m} = \mu_0 \mathbf{S}$, where $\mathbf{S} = \vec{\sigma}/2$, and $\mu_0 = eg_L/2mc$, with $\vec{\sigma}$ being the Pauli vector matrix; g_L , Landé factor; c , light velocity; and e , electric charge (for concreteness, taken to be positive). The Hamiltonian reads as

$$H(t) = -\mu_0 \mathbf{S} \cdot \mathbf{B} , \tag{41}$$

with the rotating magnetic field

$$\mathbf{B} = (B \cos \omega t) \mathbf{e}_x + (B \sin \omega t) \mathbf{e}_y , \tag{42}$$

which, without the loss of generality, can be assumed to rotate in the $x - y$ plane. The snapshot eigenvalues of Hamiltonian (41) are

$$E_1 = -\frac{1}{2} \omega_0 , \quad E_2 = \frac{1}{2} \omega_0 , \tag{43}$$

where

$$\omega_0 \equiv \mu_0 B \tag{44}$$

is the Larmor frequency. The snapshot eigenfunctions are

$$\begin{aligned}
\psi_1(t) &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{e^{i\omega t}}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \end{pmatrix} , \\
\psi_2(t) &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \frac{e^{i\omega t}}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \end{pmatrix} .
\end{aligned} \tag{45}$$

Condition (11) tells us that, if the system starts from the state $\psi_1(0)$, then its wave function $\psi(t)$ is close to the adiabatic approximation (9), for the time interval $[0, \tau]$, in the sense of Eq. (10), provided that

$$\int_0^t |\langle \psi_1(t') | \dot{\psi}_2(t') \rangle| dt' \ll 1 . \tag{46}$$

Similarly, when the system starts from $\psi_2(0)$, then the sufficient condition (11) becomes

$$\int_0^t | \langle \psi_2(t') | \dot{\psi}_1(t') \rangle | dt' \ll 1 . \quad (47)$$

From Eqs. (45), we have

$$\dot{\psi}_1(t) = \frac{i}{\sqrt{2}} \omega e^{i\omega t} \begin{pmatrix} 0 \\ 1 \end{pmatrix} , \quad \dot{\psi}_2(t) = - \frac{i}{\sqrt{2}} \omega e^{i\omega t} \begin{pmatrix} 0 \\ 1 \end{pmatrix} . \quad (48)$$

Hence

$$\langle \psi_1(t) | \dot{\psi}_2(t) \rangle = \langle \psi_2(t) | \dot{\psi}_1(t) \rangle = -\frac{i}{2} \omega . \quad (49)$$

Thus, both Eqs. (46) and (47) result in the condition

$$\omega t \ll 1 \quad (t \in [0, \tau]) . \quad (50)$$

This condition has two different representations, depending on the relation between the frequencies ω and ω_0 . If $1/\omega_0 \leq \tau$, then there exists such a time $t = 1/\omega_0$ which lies inside the interval $[0, \tau]$, which means that $\omega \ll \omega_0$. This case is summarized in the form of the conditions

$$\omega \ll \omega_0 , \quad \omega \tau \ll 1 , \quad \omega_0 \tau \geq 1 . \quad (51)$$

The opposite situation is when ω is larger or of the order of ω_0 . Then Eq. (50) is equivalent to the inequalities

$$\omega \geq \omega_0 , \quad \omega \tau \ll 1 , \quad \omega_0 \tau \ll 1 . \quad (52)$$

The first case (51) is in line with the standard understanding of the slow Hamiltonian variation, allowing for the use of the adiabatic approximation. But the second situation (52) corresponds to fast variation, including the resonance case, when ω coincides with ω_0 . For both these variants, there exists a limitation on the admissible time interval, during which the adiabatic approximation is applicable. The basic difference is that this time interval can be larger for the slow Hamiltonian variation, as compared to its fast resonance variation.

Since the considered problem allows for an exact solution, we can check whether the found conditions are really sufficient. Equation (1), under the initial condition

$$\psi(0) = c_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + c_2 \begin{pmatrix} 0 \\ 1 \end{pmatrix} , \quad (53)$$

for Hamiltonian (41), results in the solution

$$\psi(t) = b_1(t) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + b_2(t) \begin{pmatrix} 0 \\ 1 \end{pmatrix} , \quad (54)$$

in which the coefficient functions are

$$\begin{aligned} b_1(t) &= \left(c_1 \cos \frac{\Omega t}{2} + i \frac{c_1 \omega + c_2 \omega_0}{\Omega} \sin \frac{\Omega t}{2} \right) e^{-i\omega t/2} , \\ b_2(t) &= \left(c_2 \cos \frac{\Omega t}{2} - i \frac{c_2 \omega - c_1 \omega_0}{\Omega} \sin \frac{\Omega t}{2} \right) e^{i\omega t/2} , \end{aligned} \quad (55)$$

and the notation is used for the effective Rabi frequency

$$\Omega \equiv \sqrt{\omega^2 + \omega_0^2} . \quad (56)$$

Inverting relations (45) gives

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \psi_1(t) + \frac{1}{\sqrt{2}} \psi_2(t) ,$$

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{e^{-i\omega t}}{\sqrt{2}} \psi_1(t) - \frac{e^{-i\omega t}}{\sqrt{2}} \psi_2(t) . \quad (57)$$

So that expansion (6) over eigenfunctions (45) takes the form

$$\psi(t) = a_1(t) \psi_1(t) + a_2(t) \psi_2(t) , \quad (58)$$

where

$$a_1(t) = \frac{b_1(t) + b_2(t)}{\sqrt{2}} , \quad a_2(t) = \frac{b_1(t) - b_2(t)}{\sqrt{2}} . \quad (59)$$

At the initial moment of time, we have

$$b_1(0) = c_1 , \quad b_2(0) = c_2 , \quad a_1(0) = \frac{c_1 + c_2}{\sqrt{2}} , \quad a_2(0) = \frac{c_1 - c_2}{\sqrt{2}} .$$

Suppose, first, that the system starts from the eigenstate $\psi_1(0)$, when

$$\psi(0) = \psi_1(0) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \end{pmatrix} , \quad (60)$$

so that

$$a_1(0) = 1 , \quad a_2(0) = 0 , \quad c_1 = c_2 = \frac{1}{\sqrt{2}} .$$

Then Eqs. (55) yield

$$b_1(t) = \left(\cos \frac{\Omega t}{2} + i \frac{\omega + \omega_0}{\Omega} \sin \frac{\Omega t}{2} \right) \frac{e^{-i\omega t/2}}{\sqrt{2}} ,$$

$$b_2(t) = \left(\cos \frac{\Omega t}{2} - i \frac{\omega - \omega_0}{\Omega} \sin \frac{\Omega t}{2} \right) \frac{e^{i\omega t/2}}{\sqrt{2}} . \quad (61)$$

In order that the adiabatic approximation be valid for a time interval $[0, \tau]$, according to definition (10), it is necessary and sufficient that

$$| a_2(t) | \ll 1 , \quad 1 - | a_1(t) | \ll 1 \quad (62)$$

for this interval of time. From Eq. (59), we find

$$| a_2(t) |^2 = \frac{1}{4} \left| \left(1 - \cos \omega t \right) \cos \frac{\Omega t}{2} - \frac{\omega - \omega_0}{\Omega} \sin \frac{\Omega t}{2} \sin \omega t \right|^2 +$$

$$+ \frac{1}{4} \left| \left(\frac{\omega + \omega_0}{\Omega} + \frac{\omega - \omega_0}{\Omega} \cos \omega t \right) \sin \frac{\Omega t}{2} - \cos \frac{\Omega t}{2} \sin \omega t \right|^2 . \quad (63)$$

When inequality (50) holds, then Eq. (63) simplifies to

$$| a_2(t) | \simeq \left| \frac{\omega}{\Omega} \sin \frac{\Omega t}{2} \right| . \quad (64)$$

As is explained above, Eq. (50) is equivalent to one of the conditions, either (51) or (52). In both the cases, expression (64) satisfies inequality (62). Conversely, from Eqs. (62) and (63), one gets inequality (50). That is, inequality (50) is the necessary and sufficient condition for the validity of the adiabatic approximation.

Let now the system start from the eigenstate $\psi_2(0)$, which means that

$$\psi(0) = \psi_2(0) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \end{pmatrix} , \quad (65)$$

with

$$a_1(0) = 0 , \quad a_2(0) = 1 , \quad c_1 = -c_2 = \frac{1}{\sqrt{2}} .$$

Then one has

$$\begin{aligned} b_1(t) &= \left(\cos \frac{\Omega t}{2} + i \frac{\omega - \omega_0}{\Omega} \sin \frac{\Omega t}{2} \right) \frac{e^{-i\omega t/2}}{\sqrt{2}} , \\ b_2(t) &= \left(-\cos \frac{\Omega t}{2} + i \frac{\omega + \omega_0}{\Omega} \sin \frac{\Omega t}{2} \right) \frac{e^{i\omega t/2}}{\sqrt{2}} . \end{aligned} \quad (66)$$

For the adiabatic approximation to hold, in the sense of definition (10), it is necessary and sufficient that

$$| a_1(t) | \ll 1 , \quad 1 - | a_2(t) | \ll 1 . \quad (67)$$

In view of Eqs. (59), we have

$$\begin{aligned} | a_1(t) |^2 &= \frac{1}{4} \left| (1 - \cos \omega t) \cos \frac{\Omega t}{2} - \frac{\omega + \omega_0}{\Omega} \sin \frac{\Omega t}{2} \sin \omega t \right|^2 + \\ &+ \frac{1}{4} \left| \left(\frac{\omega - \omega_0}{\Omega} + \frac{\omega + \omega_0}{\Omega} \cos \omega t \right) \sin \frac{\Omega t}{2} - \cos \frac{\Omega t}{2} \sin \omega t \right|^2 . \end{aligned} \quad (68)$$

Following the same reasoning as above, we see that under inequality (50), the value of Eq. (68) becomes

$$| a_1(t) | \simeq \left| \frac{\omega}{\Omega} \sin \frac{\Omega t}{2} \right| , \quad (69)$$

which satisfies Eq. (67), because of either condition (51) or condition (52). Hence, again, inequality (50) is the necessary and sufficient condition for the applicability of the adiabatic approximation.

These examples demonstrate that inequality (11), found as a sufficient condition for the validity of the adiabatic approximation, in some cases, becomes the necessary and sufficient condition.

At the same time, the standard estimate (4) for the considered case gives

$$\left| \frac{\langle \psi_2(t) | \dot{\psi}_1(t) \rangle}{E_{21}(t)} \right| = \frac{\omega}{2\omega_0} \ll 1. \quad (70)$$

As is evident from the above consideration, this is neither necessary nor sufficient condition for the occurrence of the adiabatic approximation. This is why the situation, when inequality (70) is valid, but the adiabatic approximation is not correct, in no sense implies an inconsistency of the adiabatic theorem.

5 Discussion

A simple and general sufficient condition is derived for the validity of the adiabatic approximation in the case of quantum linear systems with arbitrary spectra and with any time variation of the related linear Hamiltonian. The adiabatic theorem is extended to the case of quantum nonlinear Hamiltonians. By considering an exactly solvable model, it is shown that the found sufficient conditions in some cases become necessary and sufficient. Contrary to this, the usually considered condition (4) is shown to be neither necessary nor sufficient.

It is important that the found conditions can be used for any type of the system spectrum, whether discrete or continuous, nondegenerate or degenerate, gapful or gapless, without or with level crossings. The temporal Hamiltonian variation can also be arbitrary, whether slow or fast, including the case of resonance transitions. The main difference between the slow and fast Hamiltonian variations is that in the former case the time interval, allowing for the validity of the adiabatic approximation, is larger than in the case of fast variation, when such a time interval can become rather short.

The summation over the spectral label n , appearing in formulas, can be explicitly realized for each particular system. There exist a variety of methods, both analytical and numerical, for evaluating such series. Moreover, for a great number of physical systems, only several lowest energy levels are of importance, which makes such systems effectively spectrally bounded. Therefore, the arising summation does not lead to principal difficulties, but is rather a technical problem, which can be appropriately addressed for each particular case.

To emphasize the difference of condition (11) from other sufficient conditions of close forms, it is worth mentioning some previous results. Thus, Tong et al. [10] considered a slow nonresonant Hamiltonian variation, for a finite-level system, with nondegenerate spectrum, without level crossings, and with a gap, separating the initial energy level from other levels. Under these restrictions, the formulated conditions are given by the set of the inequalities

$$\begin{aligned} \left| \frac{\langle \psi_j(t) | \dot{\psi}_n(t) \rangle}{E_{jn}(t)} \right| &\ll 1, \\ \int_0^\tau \left| \frac{d}{dt} \left[\frac{\langle \psi_j(t) | \dot{\psi}_n(t) \rangle}{E_{jn}(t)} \right] \right| dt &\ll 1, \\ \int_0^\tau \left| \frac{\langle \psi_j(t) | \dot{\psi}_n(t) \rangle \langle \psi_n(t) | \dot{\psi}_m(t) \rangle}{E_{jn}(t)} \right| dt &\ll 1, \end{aligned}$$

to be satisfied for any $t \in [0, \tau]$, all $n \neq j$, and any $m \neq n$. As is evident, these conditions are quite different, and are accompanied by several restrictions that are not required for Theorem 1.

Wei and Ying [28] showed that the Tong et al. conditions are valid, under the same restrictions plus the additional requirement that the Hamiltonian be real, if the following two inequalities hold:

$$\left| \frac{\langle \psi_j(t) | \dot{\psi}_n(t) \rangle}{E_{jn}(t)} \right| \ll 1 ,$$

$$\sum_{n(\neq j)} \int_0^\tau |\langle \psi_j(t) | \dot{\psi}_n(t) \rangle| dt < \text{const} ,$$

for all $n \neq j$ and $t \in [0, \tau]$. Again, the main difference is that condition (11) does not require all these restrictions, thus, being essentially more general.

Maamache and Saadi [29,30] studied a slowly varying Hamiltonian, producing no resonant transitions and enjoying a continuous nondegenerate spectrum $E_k(t)$, having no level crossings, with the parameter k inside a wave-packet range $[k_0, k_0 + \delta k_0]$, where $|\delta k_0| \ll |k|$. Their result reads as

$$\left| \int_0^\tau \exp \left\{ i \int_0^t [E_{k_0}(t') - E_k(t')] dt' \right\} \langle \psi_{k_0}(t) | \dot{\psi}_k(t) \rangle dt \right|^2 \ll 1 ,$$

$$k \in [k_0, k_0 + \delta k_0] , \quad |\delta k_0| \ll |k| .$$

A similar condition can be obtained from Eqs. (13) and (19) for the case of the continuous spectrum. However, again, we do not need the restrictions that the Hamiltonian be slowly varying and nonresonant, and the spectrum is not required to be nondegenerate and without level crossings.

For nonlinear systems, the applicability of the adiabatic approximation is substantially limited. The nonlinearity acts as an additional perturbation destroying the adiabatic evolution. If the nonlinearity is large, then the adiabatic approximation is limited by a short time interval τ , as follows from the sufficient conditions (26) to (28). When the nonlinearity is small, such that the eigenfunctions of eigenproblem (23) are almost orthogonal between each other, then the problem reduces to the case of linear Hamiltonians.

Generally speaking, nonlinear quantum systems are not good candidates for the use of the adiabatic approximation that is strongly destroyed by nonlinearity. Therefore, when considering possible physical setups for adiabatic quantum computation [16,17], it is better to keep in mind noninteracting or at least very weakly interacting systems. As examples, one could take weakly interacting trapped atoms [18-26] or cold molecules [31]. Another physical system, convenient for quantum information processing, is a collection of spins. But again, the spins should not strongly interact with each other. This imposes a severe restriction on the density of spins, since they interact through dipole forces that are long-ranged and strongly influence the spin motion [32-34]. The treatment of nonlinear systems is essentially more complicated than that of linear systems and requires a separate investigation for each particular case. For example, the validity of the adiabatic approximation for cold trapped atoms, subject to the action of an alternating trap modulation, is analyzed in Ref. [35]. The sufficient conditions, derived in the present paper, can be used for estimating the parameters of physical systems that are intended to be employed for realizing adiabatic processes, such as adiabatic quantum computing.

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